First Semester Examination
2020/2021 Academic Session

January 2021

KFE432 – Selected Topics in Physical Chemistry

Duration: 2 hours

Please check that this examination paper consists of **SEVEN (7)** pages of printed material before you begin the examination.

Instructions:

This paper has **FIVE (5)** questions. Answer not more than **FOUR (4)** questions.

Answer each question on a new page.

If a candidate answers more than four questions, only the answers to the first five questions in the answer sheet will be graded.

Appendix: Fundamental constants in physical chemistry.

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Answer **FOUR (4)** questions.

1. (a) The adsorption of N_2 onto a sample of titania powder at 77 K was found to follow the Brunauer–Emmett–Teller (BET) adsorption isotherm. A plot of the adsorption of 1.00 g titania according to the linearised BET equation gave a slope of 0.004675 g cm^{-3} and an intercept of 0.000022 g cm^{-3}. The BET equation is expressed as:

$$\frac{1}{V_{total}[(P_o/P)-1]} = \frac{C-1}{V_{mono}C}\left(\frac{P}{P_o}\right) + \frac{1}{V_{mono}C}$$

where P/P_o is the partial pressure, V_{total} is the volume adsorbed at the specific partial pressure, V_{mono} is the volume required for the monolayer adsorption and C is the BET constant. If the cross-sectional area of N_2 is 16.2×10^{-20} m^2, calculate

(i) monolayer gas adsorption capacity, V_{mono}.

(ii) specific surface area, S_{BET}.

(6 marks)

(b) The table below shows the volume of N_2 adsorbed on titania at 77 K and the respective statistical thickness.

Volume adsorbed, V_{ads} / cm^3 g^{-1} at STP	Statistical thickness, t / Å
327	3.5
334	3.9
335	4.0
338	4.2
342	4.4
352	5.0

(i) Calculate the external surface area, S_{ext}, and micropore volume, V_{micro}.

(ii) Based on your answer in question a(ii), estimate the micropore surface area, S_{micro}.

(iii) Estimate the percentage of mesoporosity.

Given that S_{ext} / m^2 g^{-1} = s × 15.47, V_{micro} / cm^3 g^{-1} = i × 0.001547, where s = slope and i = intercept of the linearised t-plot.

(13 marks)

(c) A solid sample adsorbs 0.63 mg of CO when the pressure of the gas is 36.0 kPa at 300 K. When the pressure of 4.0 kPa and temperature of 300 K are used, the mass of gas adsorbed is 0.21 mg. Calculate the values of fractional surface coverage at the two pressures if this adsorption process is well-described by the Langmuir isotherm.

(6 marks)

2. (a) Explain the phenomenon of hard water softening by zeolites in laundry industry.

(6 marks)

(b) Microporous materials such as zeolites are widely used as a solid acid catalyst in various chemical reactions including cracking, isomerisation and alkylation.

(i) Name **FOUR** properties of zeolites that make them useful in heterogeneous catalysis.

(ii) Briefly compare the properties of faujasite zeolites (X, Y and USY).

(iii) Explain why the Si/Al ratio of zeolite should not be lower than 1.

(iv) Describe how to generate the Brönsted and Lewis acid sites on zeolite surface using ion exchange technique.

(13 marks)

(c) Aluminophosphate is a zeolite-like material. Unlike aluminosilicate zeolite that has negative charge surface, it has neutral charge surface due to its primary building units made up of tetrahedral TO_4 units (T = Al or P).

(i) Calculate the charge of each tetrahedral Al and P units in an alumino-phosphate zeolite.

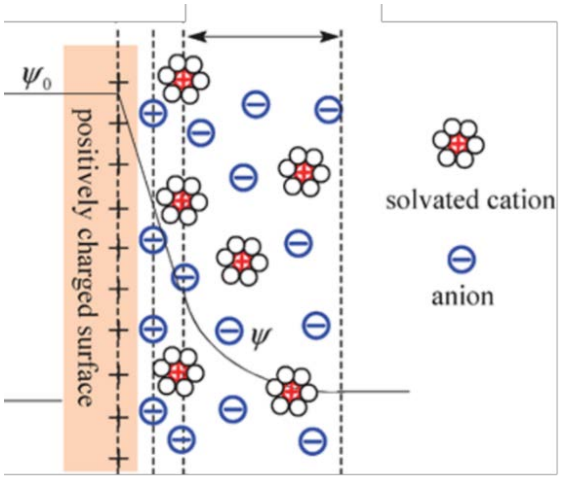
(ii) Draw the possible structure of aluminophosphate zeolite.

(6 marks)

3. (a) Describe **FOUR** mechanisms of the origin of surface charge on the preparation of stable colloid dispersion with examples.

(8 marks)

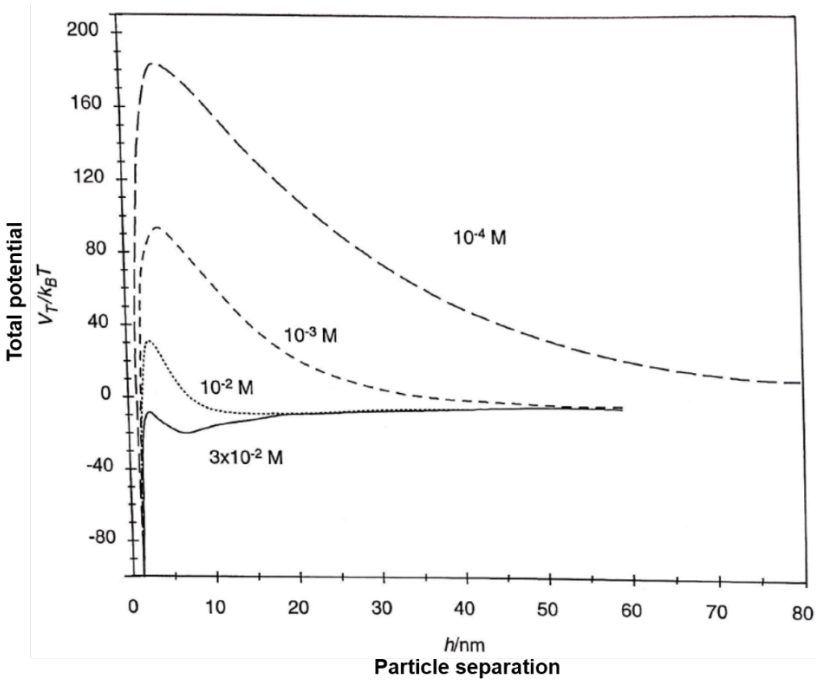
(b) Interpret possible model as shown in figure below to describe the distribution of charged surface across the solid/liquid interface.



Adapted from https://link.springer.com/article/10.1007/s10853-015-9121

(7 marks)

(c) From the graph below, examine how does the concentration of sodium chloride (NaCl) affect the total interaction potential curve.



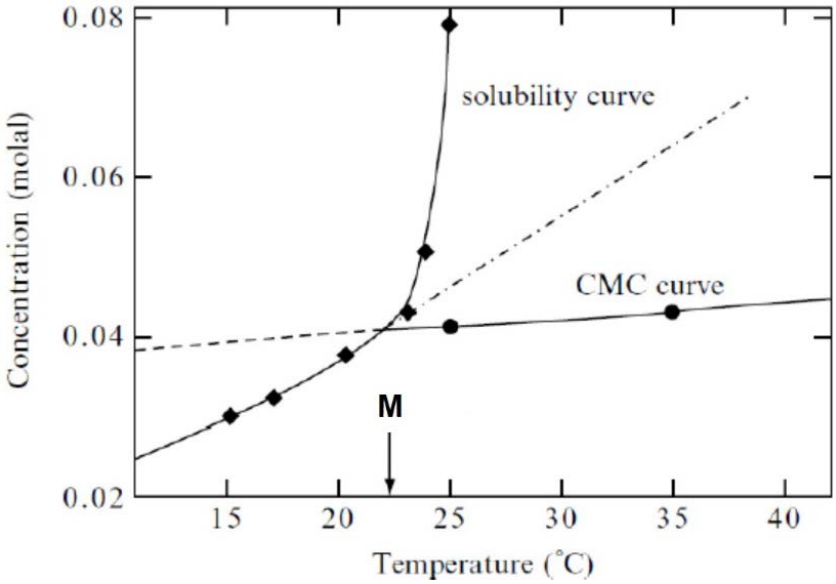
Adapted from Colloids. I. Cosgrove, T (Terence) 2010

(10 marks)

4. (a) Depending on the system composition, a surfactant molecule will undergo micellisation process to form different aggregations.

(i) Demonstrate the change in the physical properties of solutions based on the concentration of micelle forming surfactants.

(ii) Identify phenomenon M as depicted in figure below with your justification.



Adapted from https://odr.chalmers.se/bitstream/20.500.12380/154684/1/154684

(10 marks)

(b) Molecular self-assembly in surfactant solutions can be translated into a geometrical packing parameter by specific shape and size of the equilibrium aggregate.

(i) Define the concept of critical packing parameter (CPP).

(ii) Discuss **FOUR** factors that affect the prediction of CPP structure.

(iii) Calculate the CPP for non-ionic surfactant if the surface area, α_0, of a surfactant is 0.5049 nm^2 when the volume, V, and length, l_c, of the surfactant molecule are 0.2964 nm^3 and 1.415 nm, respectively.

(iv) Comment on the value obtained in b(iii).

(15 marks)

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5. (a) Composition of oil in water (o/w) emulsion are tabulated in the table below.

Surfactant	Percentage (w/w%)
Stearyl alcohol	8
Cetyl alcohol	1
Lanolin anhydrous	1
Emulsifier	4
Preserved water ad.	100

(i) Calculate total percentage and the required hydrophilic-hydrophobic balance (HLB) of the oil phase. Given that the HLB for stearyl alcohol, cetyl alcohol, and lanolin anhydrous are 15, 15 and 10, respectively.

(ii) Determine the amount (in gram) of emulsifiers of Span 80 (HLB 4.3) and Tween 60 (HLB 14.9) that used to produce 1000-g stable liquid emulsion.

(13 marks)

(b) Differentiate with illustration between the Langmuir-Hinshelwood and Eley-Rideal mechanisms for the surface catalysed reaction:

$$A\ (g) + B\ (g) \rightarrow Products\ (g)$$

(4 marks)

(c) Physisorption and chemisorption processes occur due to the repulsive and attractive forces operating between the adsorbed species and the surface of an adsorbent. Describe both phenomena using Lennard-Jones potential curve.

(8 marks)

APPENDIX

UNIVERSITI SAINS MALAYSIA
School of Chemical Sciences

General data and fundamental constants

Quantity	Symbol	Value	Power of ten	Units
Speed of light	c	2.99792458	10^{8}	m s^{-1}
Elementary charge	e	1.60218	10^{-19}	C
Faraday constant	$F = N_A e$	9.64853	10^{4}	C mol^{-1}
Boltzmann constant	k	1.38065	10^{-23}	J K^{-1}
Mass of electron	m_e	9.10938356	10^{-31}	kg
Gas constant	$R = N_A k$	8.31447		J K^{-1} mol^{-1}
		8.31447	10^{-2}	L bar K^{-1} mol^{-1}
		8.20574	10^{-2}	L atm K^{-1} mol^{-1}
		6.23637	10	LTorr K^{-1} mol^{-1}
Planck constant	h	6.62608	10^{-34}	J s
	$\hbar = h/2\pi$	1.05457	10^{-34}	J s
Avogadro constant	N_A	6.02214	10^{23}	mol^{-1}
Standard acceleration of free fall	g	9.80665		m s^{-2}

Conversion factors **Useful relation** **Unit relations**

1 eV	1.60218 x 10^{-19} J 96.485 kJ mol^{-1} 8065.5 cm^{-1}	2.303 RT/F = 0.0591 V at 25 °C	Energy	1 J = 1 kg m^2 s^{-2} = 1 A V s
			Force	1 N = 1 kg m s^{-2}
1 cal	4.184 J			
1 atm	1.013 bar 101.325 kPa 760 Torr		Pressure	1 Pa = 1 N m^{-2} = 1 kg m^{-1} s^{-2} = 1 J m^{-3}
1 cm^{-1}	1.9864 x 10^{-23} J		Charge	1 C = 1 A s
1 Å 1 L atm	10^{-10} m 101.325 J		Potential difference	1 V = 1 J C^{-1} = 1 kg m^2 s^{-3} A^{-1}

Atomic Weights

Al	26.98	C	12.01	Fe	55.85	P	30.97
Sb	121.76	Cs	132.92	Kr	83.80	K	39.098
Ar	39.95	Cl	35.45	Pb	207.2	Ag	107.87
As	74.92	Cr	51.996	Li	6.941	Na	22.99
Ba	137.33	Co	58.93	Mg	24.31	S	32.066
Be	9.012	Cu	63.55	Mn	54.94	Sn	118.71
Bi	208.98	F	18.998	Hg	200.59	W	183.84
B	10.81	Au	196.97	Ne	20.18	Xe	131.29
Br	79.90	He	4.002	Ni	58.69	Zn	65.39
Cd	112.41	H	1.008	N	14.01		
Ca	40.078	I	126.90	O	15.999		

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